

# Benzenamine, 2,4-dimethyl-

<b>Other names:</b>	1-AMINO-2,4-DIMETHYLBENZENE 2,4-DIMETHYLANILINE 2,4-Dimethylbenzenamine 2,4-Dimethylbenzeneamine 2,4-Dimethylphenylamine 2,4-XYLIDINE 2,4-Xylylamine 2-Methyl-p-toluidine 4-Amino-1,3-dimethylbenzene 4-Amino-1,3-xylene 4-Amino-3-methyltoluene 4-Methyl-o-toluidine Aniline, 2,4-dimethyl- M-XYLIDINE NSC 7640 m-4-Xylidine
<b>Inchi:</b>	InChI=1S/C8H11N/c1-6-3-4-8(9)7(2)5-6/h3-5H,9H2,1-2H3
<b>InchiKey:</b>	CZZZABOKJQXEBO-UHFFFAOYSA-N
<b>Formula:</b>	C8H11N
<b>SMILES:</b>	<chem>Cc1ccc(N)c(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	121.18
<b>CAS:</b>	95-68-1

## Physical Properties

Property code	Value	Unit	Source
af	0.4970		KDB
chl	-4655.50	kJ/mol	NIST Webbook
gf	176.08	kJ/mol	Joback Method
hf	38.93	kJ/mol	Joback Method
hfl	-88.70	kJ/mol	NIST Webbook
hfus	14.94	kJ/mol	Joback Method
hvap	47.64	kJ/mol	Joback Method
ie	7.65 ± 0.05	eV	NIST Webbook
ie	7.40 ± 0.10	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.886		Crippen Method
mcvol	109.800	ml/mol	McGowan Method

pc	4000.00	kPa	KDB
rinpol	1167.00		NIST Webbook
rinpol	196.10		NIST Webbook
rinpol	1123.10		NIST Webbook
rinpol	196.10		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1167.01		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1160.70		NIST Webbook
rinpol	1123.10		NIST Webbook
rinpol	1137.70		NIST Webbook
rinpol	1145.70		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1976.00		NIST Webbook
tb	491.20	K	NIST Webbook
tb	487.45 ± 0.50	K	NIST Webbook
tb	490.27	K	KDB
tc	714.00	K	KDB
tf	257.25 ± 1.00	K	NIST Webbook
tf	259.35 ± 0.35	K	NIST Webbook
tf	259.32 ± 0.80	K	NIST Webbook
tf	261.05 ± 0.30	K	NIST Webbook
tf	258.90 ± 1.00	K	NIST Webbook
tf	289.00	K	KDB
vc	0.405	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.15	J/mol×K	679.65	Joback Method
cpg	228.80	J/mol×K	491.61	Joback Method
cpg	240.98	J/mol×K	529.22	Joback Method
cpg	252.48	J/mol×K	566.83	Joback Method
cpg	263.33	J/mol×K	604.43	Joback Method
cpg	273.54	J/mol×K	642.04	Joback Method
cpg	292.16	J/mol×K	717.26	Joback Method
hvapt	61.30 ± 0.60	kJ/mol	317.00	NIST Webbook
hvapt	55.50	kJ/mol	434.00	NIST Webbook
hvapt	56.90	kJ/mol	405.50	NIST Webbook
rhol	969.46	kg/m <sup>3</sup>	293.10	KDB

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44845e+01
Coeff. B	-4.09072e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	522.53

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.53270e+02
Coeff. B	-1.27469e+04
Coeff. C	-2.03281e+01
Coeff. D	1.36820e-05
Temperature range (K), min.	294.15
Temperature range (K), max.	473.15

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>KDB:</b>	<a href="https://www.thermo.com/files/research/kdb/mol/mol1306.mol">https://www.thermo.com/files/research/kdb/mol/mol1306.mol</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C95681&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95681&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1306">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1306</a>

# Legend

<b>af:</b>	Acentric Factor
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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